Critical Exponents in a Quantum Phase Transition of an Anisotropic 2D Antiferromagnet

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I use the two-step density-matrix renormalization group method to extract the critical exponents β and ν in the transition from a Néel $Q = (\pi, \pi)$ phase to a magnetically disordered phase with a spin gap. I find that the exponent β computed from the magnetic side of the transition is consistent with that of the classical Heisenberg model, but not the exponent $z\nu$ computed from the disordered side. I also show the contrast between integer and half-integer spin cases.

There is current interest in studying quantum phase transitions (QPT) in frustrated quantum systems [1]. An interesting phenomenon generated by frustration is the dimensional reduction recently observed in the Bose-Einstein condensation QPT of $BaCuSi_2O_6$ [2]. In addition to their connection to real materials, these 2D models could be an example of systems where the conventional Landau-Ginzburg-Wilson (LGW) approach to phase transitions may fail. Of particular interest is the transition from an antiferromagnet (AFM) to a disordered phase with a spin gap and short-range magnetic correlations known as a valence bond crystal (VBC). A very fruitful approach to the study of these transitions relies on to the mapping of the Heisenberg model to the non-linear sigma (NLσ) model[9, 10]. If the Berry phase terms are neglected at the transition as suggested in Ref.[9], the critical behavior of the quantum 2D model is identical to that of the NLσ model. However, the Berry phase effects are absent only in the AFM phase; they are important in the disordered phase and they might well modify the critical exponents of the 2D Heisenberg model as suggested in Ref.[10].

The transition from an AFM to a spin gap in the 2D Heisenberg model was studied in Ref.[3] by the Quantum Monte Carlo (QMC) method. It was concluded that this transition belongs to the universality class of the $O(3)$ classical Heisenberg model as may be expected from the $NL\sigma$ mapping. In this study, the disordered phase was generated by the explicit dimerization of the bonds. This would support the view of Ref.[9] that Berry phase effects do not affect the transition. But due to the minus sign problem, the important case of transition driven by frustration cannot be studied by the QMC method. Hence, it remains to be seen whether frustration merely brings some technical complication, as would suggest the hypothesis that the universality class does not depend on the detail of the Hamiltonian, or it can drive the transition to another universality class.

There is also a more general interest in studying frustration induced transitions. The conventional approach to quantum phase transitions is to use the path integral formalism which maps quantum phase transitions in dimension d to classical transitions in dimension $d+1$ to which the machinery of the Landau-Ginzburg-Wilson theory is then applied. However, this mapping is fraught with difficulty in some important situations. For some experimentally relevant quantum mechanical models, the corresponding classical functional integrals have non-positive or even complex valued Boltzmann weights. This would suggest in such cases that the quantum transition does not have a classical equivalent. It is thus important to study the quantum models directly. But the direct study of such quantum mechanical models has proven to be a formidable challenge to condensed-matter theorists both numerically and analytically. In particular, the QMC method, which in its formulation uses this quantum-classical mapping, is at present unable to address these issues because of the non-positive values of the effective Boltzmann weights. This state of matter has stalled progress in the understanding of QPT.

In a recent publication [4], it has been shown that 2D problems may be attacked by a chain perturbation theory method. This method called the two-step DMRG has recently been applied to study quantum phase transitions induced by frustration in two dimensions. The two-step DMRG is not a simple Green's function perturbation expansion which is known to fail in situations where quantum fluctuations are important. It is rather a perturbation expansion on the reduced Hamiltonian. It thus retains the full low-energy many-body dynamics of the original problem. The two-step method has the ability to reach an ordered phase when it exists. In this letter, we report the computation of the critical exponents in the important case of the transition from an AFM to a VBC induced by frustration for $S = 1$. Such a transition was suggested in Ref.[12] from a large N analysis and found in an anisotropic 2D Heisenberg model with $S = 1$ in Ref.[4]. In addition we highlight the difference between integer spin and half-integer spin systems by comparing the case of $S = \frac{3}{2}$ to that of $S = 1$.

I study the following Heisenberg model on the anisotropic square lattice:

$$H = J_{\parallel} \sum_{i,l} \mathbf{S}_{i,l}\mathbf{S}_{i+1,l} + J_{\perp} \sum_{i,l} \mathbf{S}_{i,l}\mathbf{S}_{i,l+1}$$

$$+J_d \sum_{i,l} (\mathbf{S}_{i,l}\mathbf{S}_{i+1,l+1} + \mathbf{S}_{i+1,l}\mathbf{S}_{i,l+1}), \quad (1)$$

where $S = 1$, $J_\parallel$ is the in-chain exchange parameter and is set to 1; $J_\perp$ and J_d are respectively the transverse and diagonal interchain exchanges.

In the TSDMRG, we start by applying the DMRG to a single chain for which we obtain the low energy eigenvalues ϵ_n and eigenvectors $|\phi_n\rangle$. Then the Hamiltonian (1) is projected unto the tensor product $|\Phi_{\parallel[n]}\rangle = |\phi_{n_1}\rangle|\phi_{n_2}\rangle...|\phi_{n_L}\rangle$ yielding the effective low energy Hamiltonian

$$\tilde{H} \approx \sum_{[n]} E_{\parallel[n]} |\Phi_{\parallel[n]}\rangle\langle\Phi_{\parallel[n]}| + J_\perp \sum_{il} \tilde{\mathbf{S}}_{i,l}\tilde{\mathbf{S}}_{i,l+1} + J_d \sum_{il} \tilde{\mathbf{S}}_{i,l}\tilde{\mathbf{S}}_{i+1,l+1} + \tilde{\mathbf{S}}_{i+1,l}\tilde{\mathbf{S}}_{i,l+1}, \quad (2)$$

where $E_{\parallel[n]}$ is the sum of eigenvalues of the different chains, $E_{\parallel[n]} = \sum_l \epsilon_{n_l}$; $\tilde{\mathbf{S}}_{i,l}$ are the renormalized matrix elements in the single chain basis. They are given by $\tilde{\mathbf{S}}_{i,l}^{n_l,m_l} = \langle\phi_{n_l}|\mathbf{S}_{i,l}|\phi_{m_l}\rangle$. Since the diagonalization has been made in the direction of the chains, the effective Hamiltonian(2) is 1D. I again use the DMRG to obtain its spectrum.

The TSDMRG has been extensively checked[4, 6], and is variational. It is controlled by two parameters m_1 and m_2 which are the numbers of states kept during the first and second step respectively. m_1 should be large enough so that not only the ground-state energy of a single chain l but all the ϵ_{n_l} and ϕ_{n_l} retained to be used during the second step are accurate enough. And, m_2 should be large enough so that $J_\perp,\ J_d \ll \epsilon_{n_l} - \epsilon_{0_l}$. For instance for $S = \frac{1}{2}$, we find that the ground-state energy per site of a 16×17 system evolves from -0.43481 when $(m_1, m_2) = (128, 80)$ to -0.43681 when $(m_1, m_2) = (256, 96)$ these energies are to be compared to the QMC energy -0.43529. It may be argued that despite this accuracy in the ground-state energy, the TSDMRG would not couple the chains effectively and thus may essentially retain 1D physics. This would result in a rapid decay of the tranverse spin-spin correlation function $C_\perp$. To counter this argument we show in TableI $C_\perp$ for the 16×17 systems. When m_1 and m_2 are large enough, there is no spurious decay of the correlation of the TSDMRG, they appear to decay even slower than the QMC ones. Hence, although it starts from an isolated chain, the TSDMRG is able to describe the 2D regime.

In Ref([5]), it was found that as J_d moves towards the maximally frustrated point $J_d \approx J_\perp/2$ the 2D system progressively relax to nearly disconnected chains. At this point, the ground state energy is nearly equal to that of disconnected chains, the transverse spin-spin correlations decay exponentially, and the transverse bond-strength is equal to zero up to the numerical accuracy. Hence, for integer spins, the nature of the ground state is determined

l	$(m_1, m_2) = (128, 80)$	$(m_1, m_2) = (256, 96)$	QMC
1	-0.02116	-0.03022	-0.02533(1)
2	0.00726	0.01088	0.00854(1)
3	-0.00320	-0.00572	-0.00399
4	0.00147	0.00320	0.00201
5	-0.00078	-0.00186	-0.00105
6	0.00030	0.00108	0.00056
7	-0.00013	-0.00063	-0.00030
8	0.00006	0.00036	0.00015

TABLE I: Transverse correlation $C_\perp(l)$ for a 16×17 system with $J_\perp = 1$ and $J_d = 0$ of two sets of TSDMRG parameters against QMC. The origin is taken at the middle of the lattice.

by the competition between $J_{eff} = J_\perp - 2J_d$ which favors a magnetic phase and the 1D Haldane gap Δ_H which favors a disordered phase. For half-integer spin systems, the system would be ordered everywhere except exactly at the maximally frustrated point where it would be critical.

This behavior predicted by TSDMRG may be found analytically by applying the Haldane [7, 8] mapping of the Heisenberg model to the non-linear σ-model. I write

$$\hat{\mathbf{\Omega}}_{jl} = \eta_j \hat{\mathbf{n}}_{jl}\sqrt{1 - \mathbf{m}_{jl}^2} + \mathbf{m}_{jl}, \quad (3)$$

where $\hat{\Omega}_{jl}.\mathbf{S}_j l|\hat{\Omega}_{jl}\rangle = S|\hat{\Omega}_{jl}\rangle$ is a spin-coherent state, $\hat{n}_{jl}$ is the local Néel field, η_i is the sublattice modulation, $\mathbf{m} = \frac{v_0 \mathbf{l}}{S\hbar}$ and $\mathbf{l}$ describes the ferromagnetic fluctuations about the Néel order and v_0 is the unit cell volume. Keeping only up to second order terms in $\mathbf{m}_{jl}$, the Hamiltonian(1) becomes,

$$H' = \sum_l \int dx[\rho_s(\partial_x \hat{\mathbf{n}}_l(x))^2 + \chi^{-1}\mathbf{m}_l^2(x) - (J_\perp - 2J_d) \times \hat{\mathbf{n}}_l(x).\hat{\mathbf{n}}_{l+1}(x) + (J_\perp + 2J_d)\mathbf{m}_l(x).\mathbf{m}_{l+1}(x)], \quad (4)$$

where $\rho_s = -\frac{S^2}{2Nv_0}\sum_{jj'} \eta_j\eta'_j(x_j - x_{j'})^2$ and $\chi^{-1} = \frac{v_0}{2N\hbar^2}\sum_{jj'}(1 - \eta_j\eta_{j'})$ are respectively the spin stiffness and the inverse susceptibility along the chains. As usual, one must add the Berry phase term,

$$S_B = S\sum_{jl} \eta_j \omega[\hat{\mathbf{n}}_{jl}] + \sum_l \int dx \mathbf{m}_l(x).\frac{\partial \hat{\mathbf{n}}_l(x)}{\partial t} \times \hat{\mathbf{n}}_l(x). \quad (5)$$

Then, writing the total action resulting from H' and S_B and performing the integration over the fields $\mathbf{m}_l(x)$ with the constraint $\hat{\mathbf{n}}_l(x).\mathbf{m}_l(x) = 0$ yields, at the maximally frustrated point, the following effective action:

$$S_E = \sum_l \int dx \rho_s(\partial_x \hat{\mathbf{n}}_l^2(x) + K_{ll'}(\frac{\partial \hat{\mathbf{n}}_l}{\partial t} \times \hat{\mathbf{n}}_l).(\frac{\partial \hat{\mathbf{n}}_{l'}}{\partial t} \times \hat{\mathbf{n}}_{l'}), \quad (6)$$

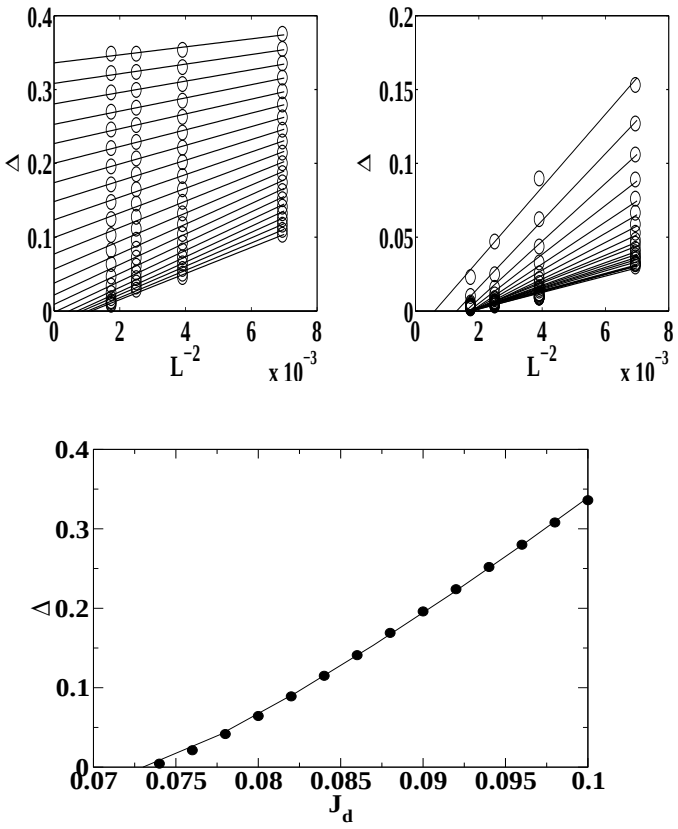

FIG. 1: TOP: Gaps for $S = 1$ (left) and $S = \frac{3}{2}$ (right) for $J_\perp = 0.2$ and for J_d ranging from $J_d = 0.06$ (bottom) to $J_d = 0.1$ (top) with the step $\delta J_d = 0.02$. BOTTOM: Extrapolated gap for $S = 1$ and for the same values of J_d as above.

where $K^{-1}_{ll'} = \delta_{ll'}\chi^{-1} + (J_\perp + 2J_d)\delta_{ll'+1}$. Hence, to the leading order, at $J_d = J_\perp/2$, the chains are only coupled by terms originating from the Berry phase on each chain. Therefore as found numerically [4], unlike the magnetic case where S does not play any role, the physics of the 2D system near the maximally frustrated point will strongly depends on the 1D physics, i.e., whether S is integer or half-integer as found numerically.

For relatively small $J_\perp$, the eventual magnetic order parameter is roughly $m \propto \sqrt{J_\perp}$ for $J_d = 0$ [11] and m will get even smaller when $J_d \neq 0$. For this reason, the critical behavior of $S = \frac{1}{2}$ systems is very difficult to study. I therefore choose $S = 1$ and $S = \frac{3}{2}$ for which m is larger and could be extrapolated to from lattice sizes not too large. The simulations were done on $L \times (L+1)$ systems with $L = 8$, 12, 16, 20 and 24. I use the periodic boundary conditions (PBC) in the direction parallel to the chains and open boundary conditions (OBC) in the transverse direction. I kept a maximum of $m_1 = 243$ states during the first step. I targeted the spin sectors $S^z = 0, \pm 1, \pm 2$. The maximum truncation error during this step was $\rho_1 = 9 \times 10^{-6}$. During the second step I kept a maximum of $m_2 = 100$ states. During the second step I targeted two states $S^z = 0, 1$. The truncation error was about 5×10^{-4} in the magnetic phase. It dropped to 6×10^{-7} in the disordered phase. The TSDMRG is thus at its best in the vicinity of the transition and in the disordered phase.

In Fig.1, I show the finite size gap Δ for $S = 1$ and $S = \frac{3}{2}$. In all cases, $J_\perp = 0.2$ and J_d is varied from 0.06 to 0.1. The $S = 1$ and $S = \frac{3}{2}$ show a striking difference. For $S = 1$, starting from 0.06 where the system is gapless and decay to 0 faster than L^{-1}, a gap opens around $J_d = 0.073$. This gap opening signals a transition from an AFM to a magnetically disordered phase. On the other hand, the $S = \frac{3}{2}$ system remains gapless for all values of J_d. The fact that $S = \frac{3}{2}$ remains gapless makes the transition at the maximally frustrated point quite difficult to study because long-range order vanishes only at the critical point an beyond this point, the Néel phase $(\pi, 0)$ sets in. This is complicated by the fact that for finite systems with OBC, the maximally frustrated point is not exactly at $J_d = J_\perp/2$ [4]. Hence, the critical behavior could only be analyzed for $S = 1$. I show the in Fig.1 extrapolated gap as function of J_d for $S = 1$. Δ vanishes at $J_{d_c} \approx 0.073$. Taking as granted the large N prediction that the transition is of second order, I extracted the critical exponent $z\nu = 1.205$ ($\Delta \propto (J_d - J_{d_c})^{z\nu}$). Hence, Hamiltonian (1) does not belong to the universality class of the classical $O(3)$ Heisenberg model for which $z\nu = 0.7048 \pm 0.0030$.

The center-to-end spin-spin correlation function $C_L = \frac{1}{3}\langle \mathbf{S}_{L/2,L/2+1}\mathbf{S}_{L,L/2+1}\rangle$ is shown in Fig.2. C_L is also dependent on S. For $S = 1$, C_L first decays slower than L^{-1} and extrapolates to a finite value for small J_d, then decays faster than L^{-1} for larger J_d, where it extrapolates to 0. For $S = \frac{3}{2}$ for all values of the coupling studied, C_L extrapolates to a finite value. The behavior of the magnetization $m = \sqrt{3C_\infty}$ shown in Fig.2 is consistent with that of Δ. For $S = 1$, starting from the AFM phase for $J_d = 0.06$, m vanishes around $J_d \approx 0.076$. The best fit to data yields the exponent $m \propto (J_{d_c} - J_d)^\beta$, $\beta = 0.3653$ which is in good agreement with that of the classical Heisenberg model $\beta = 0.3639 \pm 0.0035$. By contrast, m for $S = \frac{3}{2}$ extrapolates to a finite value for all values of $J_d \lesssim 0.1$. This result, with that seen for Δ, contradicts the large N prediction that there is a VBC phase in this regime for $S = \frac{3}{2}$ as well. Ultimately, I find that long-range order vanishes when $J_d \approx 0.11$ for all L studied and, immediately, the systems jumps to the Néel phase with $Q = (\pi, 0)$. The critical behavior for $S = \frac{3}{2}$ was quite difficult to study. This is because, close enough to the critical point, for a fixed J_d, starting from the Néel phase with $Q = (\pi, \pi)$, the system evolves to the $Q = (\pi, 0)$ Néel phase at larger L. For this reason, the extrapolations cannot be reliably made.

A previous Monte Carlo simulation [3] for a Heisenberg model with $S = 1/2$ on the CaV_4O_9 lattice with

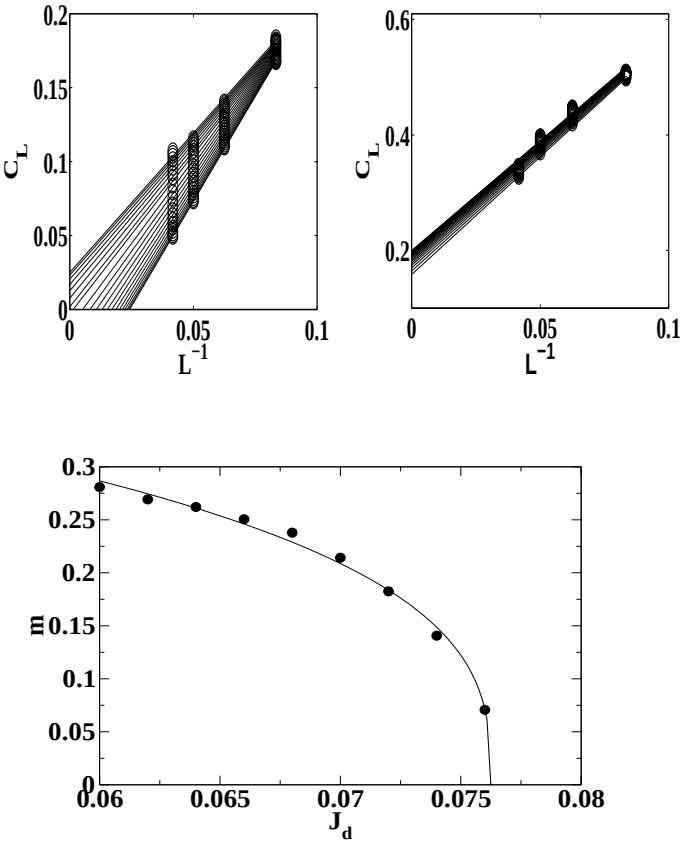

FIG. 2: TOP: End-to-center correlation C_L for $S = 1$ (left) and $S = \frac{3}{2}$ (right) for $J_\perp = 0.2$ and J_d ranging from $J_d = 0.06$ (bottom) to $J_d = 0.1$ (top) with the step $\delta J_d = 0.02$. BOTTOM: Extrapolated magnetization for $S = 1$ and for the same values of J_d as above.

found $\nu = 0.685$ and $\beta = 0.345$. These exponents are in agreement with the classical Heisenberg model within statistical errors. It is not definitive whether the QMC results are in contradiction with my results. In the QMC study, following the assumption that critical exponents are the same in either side of the transition, ν was calculated from the ordered side through the spin stiffness $\rho_s \propto (g_c - g)^{z\nu}$. One of the standard results of the classical critical phenomena is that the critical exponents of the region above the transition are identical to those below the transition. It is not however obvious that this result extends to quantum phase transitions. From the QMC results and mine, it seems that the exponents found for model (1) violate this LGW classical behavior. The exponents in the AFM phase verify the relation $(d + z - 2 + \eta)\nu = 2\beta$. Since $d = 2$, if I assume that the critical exponent on either side of the transition are identical, I may use $z\nu$ found in the disordered case in this relation. Then, it is clear the above relation between critical exponents is not satisfied given that η is predicted to be small, $\eta = 0.0033$ for the classical Heisenberg model. This violation is possibly related to a dimensional reduction at the critical point. At the maximally frustrated point the bond strength in the transverse direction vanishes. Hence, the system is effectively 1D. It could be that this 1D physics emerges at the critical point. An alternative possibility which is consistent with the small difference find in J_{d_c} from Δ and from m, is that the transition is of first order and there is a narrow region of coexistence of the two phases.

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